

REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. <b>PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.</b>					
1. REPORT DATE (DD-MM-YYYY) 02-03-2010		2. REPORT TYPE Final Performance Report		3. DATES COVERED (From - To) 6/1/2009-11/30/2009	
4. TITLE AND SUBTITLE  The Fourteenth International Meeting on Time-Resolved Vibrational Spectroscopy (TRVS XIV)				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER FA9550-09-1-0473	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)  Andrei Tokmakoff, Professor of Chemistry, Massachusetts Institute of Technology				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  Massachusetts Institute of Technology Department of Chemistry 77 Massachusetts Avenue Cambridge, MA 02139				8. PERFORMING ORGANIZATION REPORT NUMBER  OSP # 2742522	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)  Air Force Office of Scientific Research				10. SPONSOR/MONITOR'S ACRONYM(S)  AFOSR	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION / AVAILABILITY STATEMENT A					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT  This grant supported the operation of the Fourteenth International Meeting on Time-Resolved Vibrational Spectroscopy (TRVS XIV), which was held May 9-14, 2009 in Meredith New Hampshire. The conference drew 116 participants and featured 60 oral presentations and 55 poster presentations. AFOSR supported the travel of 9 scientists selected for oral presentations at the conference, in addition to some operating expenses.					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER (include area code)

Final Performance Report

submitted to the

Air Force Office of Scientific Research  
875 North Randolph Street  
Suite 325, Room 3112  
Arlington, VA 22203-1768

by

Massachusetts Institute of Technology  
Department of Chemistry  
77 Massachusetts Avenue  
Cambridge, MA 02139

for

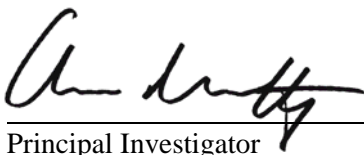
**THE FOURTEENTH INTERNATIONAL MEETING ON TIME-RESOLVED  
VIBRATIONAL SPECTROSCOPY (TRVS XIV)**

Principal Investigator:

Andrei Tokmakoff  
Professor of Chemistry  
Massachusetts Institute of Technology  
Room 6-213  
Cambridge, MA 02139  
Tel: 617-253-4503  
Fax: 617-253-7030  
e-mail: tokmakof@MIT.edu

Project Manager: Dr. Michael Berman

Grant Number: FA9550-09-1-0473



Principal Investigator  
Andrei Tokmakoff  
Professor of Chemistry

March 2, 2010  
(date)

**Abstract:** This grant supported the operation of the Fourteenth International Meeting on Time-Resolved Vibrational Spectroscopy (TRVS XIV), which was held May 9-14, 2009 in Meredith New Hampshire. The conference drew 116 participants and featured 60 oral presentations and 55 poster presentations. AFOSR supported the travel of 9 scientists selected for oral presentations at the conference, in addition to operating expenses.

The Fourteenth International Meeting on Time-Resolved Vibrational Spectroscopy (TRVS XIV) was held May 9-14, 2009 in Meredith, New Hampshire at the Inns and Spa at Mill Falls. This was the fourteenth in a series of biennial conferences covering the use of advanced vibrational spectroscopy for the use of studying time-dependent molecular processes in chemistry, physics and biology. This conference was widely considered by attendees to be one of the best conferences of the series, owing to a prominent list of invited speakers, a variety of exciting new research directions, international participation, and a significant participation by junior scientists. The conference drew 116 participants and featured 60 oral presentations (16 invited) and 55 poster presentations.

The topics of the conference included:

- Dynamics of liquids, solids, interfaces, and nanostructured materials
- TRVS in molecular biophysics and photobiology
- Chemical, vibrational, and hydrogen bonding dynamics
- Proton and electron transfer studies for energy conversion and storage
- Multidimensional vibrational spectroscopy: IR, Raman, and THz
- Single molecule vibrational spectroscopy
- Theoretical and computational spectroscopy

A full listing of the conference program and the conference attendees is attached. A book of abstracts featuring one page research synopses was distributed to conference participants. Full details of the conference program and organization are available on the conference web site: <http://web.mit.edu/trvs/>.

Funding for the conference operating costs was split roughly equally between government agencies (AFOSR, DOE), Boston area universities (MIT, Northeastern, Boston University), and company sponsors. Scientific organization was headed by Andrei Tokmakoff, with administrative assistance by Anne Hudson, Krupa Ramasesha, and Becky Nicodemus at MIT.

Most of the logistics for the conference were handled by MIT Conference Services. This AFOSR grant was used to support \$3000 in operating costs and \$4500 in travel grants to partially support the travel of young scientists giving oral presentations at the meeting. The travel support was distributed as follows:

Dave McCammant	Univ. of Rochester	\$500
Munira Khalil	Univ. of Washington	\$500
John Asbury	Penn State Univ.	\$500
Aaron Massari	Univ. of Minnesota	\$500
Kevin Kubarych	Univ. of Michigan	\$500
Ken Eisenthal	Columbia Univ.	\$500
Paul Champion	Northeastern Univ.	\$500
Gilad Haran	Weizmann Institute	\$500
Mariangela Di Donato	Univ. Amsterdam	\$500

The organizing committee thanks the AFOSR for their generous support of this highly successful conference.

## TRVS Final Attendees List

Esben Ravn	Andresen	Physikalisch-chemisches Institut	Switzerland	e.andresen@pci.uzh.ch
Stefan	Arnold	Martin-Luther-Universität Halle-Wittenberg	Germany	st.arnold@gmx.de
John	Asbury	Penn State University	United States	jasbury@psu.edu
George	Atkinson	University of Arizona	United States	atkinsonga@mindspin.org
Ellen	Backus	Amolf	Netherlands	backus@amolf.nl
Carlos	Baiz	University of Michigan	United States	jrieger@umich.edu
Huib	Bakker	FOM-AMOLF	Netherlands	bakker@amolf.nl
Artem	Bakulin	University of Groningen	Netherlands	a.a.bakulin@rug.nl
Andreas	Barth	Stockholm University	Sweden	barth@dbb.su.se
Alexander	Benderskii	Wayne State University	United States	alex@chem.wayne.edu
Mischa	Bonn	FOM-Institute AMOLF	Netherlands	bonn@amolf.nl
Eric	Borguet	Temple University	United States	eborguet@temple.edu
Tiago	Buckup	Philipps-Universität Marburg	Germany	buckup@staff.uni-marburg.de
Paul	Champion	Northeastern University	United States	champ@neu.edu
Minhaeng	Cho	Korea University	Korea, Republic of	mcho@korea.ac.kr
Susan	Dexheimer	Washington State University	United States	dexheimer@wsu.edu
Mariangela	Di Donato	Vrije Universiteit Amsterdam	Netherlands	didonat@few.vu.nl
Feng	Ding	Department of Chemistry and Biochemistry	United States	fding@umd.edu
Dana	Dlott	University of Illinois at Urbana-Champaign	United States	dclott@illinois.edu
Kenneth	Eisenthal	columbia university	United States	kbe1@columbia.edu
Thomas	Elsaesser	Max-Born-Institute	Germany	elsaesser@mbi-berlin.de
Michael	Fayer	Stanford University	United States	fayer@stanford.edu
Christian	Frischkorn	Freie Univ. Berlin	Germany	christian.frischkorn@physik.fu-berlin.de
Ziad	Ganim	MIT, Department of Chemistry	United States	ziadg@mit.edu
Sean	Garrett-Roe	University of Zurich	Switzerland	s.garrett-roel@pci.uzh.ch
Marloes	Groot	VU University Amsterdam	Netherlands	ml.groot@few.vu.nl
Scott	Gruenbaum	Cornell University	United States	smg68@cornell.edu
Karin	Haiser	LMU Munich	Germany	karin.haiser@physik.uni-muenchen.de
Hiro-o	Hamaguchi	The University of Tokyo	Japan	hhama@chem.s.u-tokyo.ac.jp
Gilad	Haran	Weizmann Institute of Science	Israel	gilad.haran@weizmann.ac.il
Charles	Harris	University of California	United States	cbharris@berkeley.edu
Karin	Hauser	University of Frankfurt	Germany	hauser@biophysik.uni-frankfurt.de
Patrick	Hayes	Northwestern University	United States	patrickhayes@u.northwestern.edu
Edwin	Heilweil	NIST	United States	ejh@nist.gov
Ismael	Heisler	University of East Anglia	United Kingdom	i.heisler@uea.ac.uk
Jan	Helbing	University of Zurich	Switzerland	j.helbing@pci.uzh.ch
Robin	Hochstrasser	University of Pennsylvania	United States	hochstra@sas.upenn.edu
Andrew	Horning	Massachusetts Institute of Technology	United States	ahorning@mit.edu
Anne	Hudson	MIT Dept. of Chemistry	United States	amh@mit.edu
Adriana	Huerta Viga	University of Amsterdam	Netherlands	a.huertaviga@uva.nl
Neil	Hunt	Dept of Physics, University of Strathclyde	United Kingdom	nhunt@phys.strath.ac.uk
Koichi	Iwata	Gakushuin University	Japan	iwata@chem.s.u-tokyo.ac.jp
Thomas	Jansen	University of Groningen	Netherlands	t.l.c.jansen@rug.nl
Kevin	Jones	Massachusetts Institute of Technology	United States	kcj@mit.edu
Valeriy	Kasyanenko	Tulane University/Department of Chemistry	United States	vkasyane@tulane.edu
Timothy	Keiderling	University of Illinois at Chicago	United States	tak@uic.edu
Munira	Khalil	University of Washington	United States	mkhalil@chem.washington.edu
Takayoshi	Kobayashi	University of Electro-Communications	Japan	kobayashi@ils.uec.ac.jp
Christopher	Konek	Indian Head, NSWC	United States	christopher.konek.ctr@navy.mil
Carsten	Kötting	Ruhr-Universität Bochum	Germany	carsten.koetting@rub.de
Kevin	Kubarych	University of Michigan	United States	jrieger@umich.edu
Damien	Laage	Ecole Normale Supérieure - CNRS	France	damien.laage@ens.fr
Bernhard	Lang	University of Geneva	Switzerland	bernhard.lang@unige.ch
Joshua	Lessing	MIT chemistry dept	United States	jlessing@mit.edu
Tianquan	Lian	Emory University	United States	tlian@emory.edu
Yu-Shan	Lin	UW-Madison	United States	lin5@wisc.edu
Roger	Loring	Cornell University	United States	rfl2@cornell.edu
H Peter	Lu	Bowling Green State University	United States	hplu@bgsu.edu
Michael	Lynch	University of Washington	United States	mlynch6@u.washington.edu
Aritra	Mandal	Massachusetts institute of Technology	United States	aritra@mit.edu
Aaron	Massari	University of Minnesota	United States	massari@umn.edu

Richard	Mathies	University of California, Berkeley	United States	rich@zinc.cchem.berki
Kamila	Mazur	University of East Anglia	United Kingdom	k.mazur@uea.ac.uk
David	McCamant	University of Rochester	United States	mccamant@chem.rocl
Shawn	McGrane	Los Alamos National Laboratory	United States	mcgrane@lanl.gov
Stephen	Meech	University of East Anglia	United Kingdom	s.meech@uea.ac.uk
Michael	Mross	Vermont Photonics Technologies Corp.	United States	mmross@vermontpho
Shaul	Mukamel	University of California, Irvine	United States	smukamel@uci.edu
Keith	Nelson	MIT	United States	kanelson@mit.edu
Karsten	Neumann	Goethe University	Germany	kneumann@theochem
Erik T.J.	Nibbering	Max Born Institut	Germany	nibberin@mbi-berlin.c
Rebecca	Nicodemus	MIT	United States	nicodemu@mit.edu
Tomonori	Nomoto	Kobe University	Japan	nomoto@kobe-u.ac.jp
Jennifer	Ogilvie	University of Michigan	United States	jogilvie@umich.edu
Junichi	Ono	Kyoto University	Japan	ono@kuchem.kyoto-u
Jeffrey	Owrutsky	Naval Research Laboratory	United States	jeff.owrutsky@nrl.nav
Alexander	Paarmann	University of Toronto	Canada	alexis@lphys.chem.utc
Matthijs	Panman	Universiteit van Amsterdam	Netherlands	m.r.panman@uva.nl
Chunte	Peng	MIT	United States	sampeng@mit.edu
Poul	Petersen	MIT	United States	poul@mit.edu
Lukasz	Piatkowski	FOM Institute - AMOLF	Netherlands	piatkowski@amolf.nl
Maxim	Pshenichnikov	University of Groningen	Netherlands	m.s.pchenitchnikov@r
Krupa	Ramasesha	Massachusetts Institute of Technology	United States	krupa_r@mit.edu
Nadja	Regner	LMU Munich	Germany	nadja.regner@physik.u
Roberto	Righini	LENS, University of Florence	Italy	righini@lens.unifi.it
Sean	Roberts	Massachusetts Institute of Technology	United States	seanr@mit.edu
Igor	Rubtsov	Tulane University	United States	irubtsov@tulane.edu
Sanford	Ruhman	Hebrew University	Israel	sandy@fh.huji.ac.il
Daniel	Shaw	University of Amsterdam	Netherlands	j.d.shaw@uva.nl
Sergey	Shilov	Bruker	United States	jrs@brukeroptics.com
Rintaro	Shimada	The University of Tokyo	Japan	rintaro@chem.s.u-tok
James	Skinner	University of Wisconsin	United States	skinner@chem.wisc.ec
Kyryl	Solntsev	Georgia Tech	United States	solntsev@gatech.edu
Andreas	Stahl	Free University Amsterdam	Netherlands	adstahl@few.vu.nl
Guillaume	Stirnemann	Ecole normale superieure	France	guillaume.stirnemann(
Tahei	Tahara	RIKEN	Japan	tahei@riken.jp
Rutger	Timmer	AMOLF	Netherlands	r.timmer@amolf.nl
Andrei	Tokmakoff	MIT	United States	tokmakof@mit.edu
Hajime	Torii	Shizuoka University	Japan	torii@ed.shizuoka.ac.jj
David	Turton	University of Strathclyde	United Kingdom	david.turton@phys.str
Richard	Van Duyne	Northwestern University	United States	vanduyne@northwest
Jasper	Van Thor	Imperial College London	United Kingdom	j.vanthor@imperial.ac
Alipasha	Vaziri	HHMI	United States	rewiss@janelia.hhmi.c
Peter	Vohringer	University of Bonn	Germany	p.voehringer@uni-bon
Dan	Weidinger	Naval Research Laboratory	United States	daniel.weidinger.ctr@
Wolfgang	Werncke	Max-Born-Institut	Germany	werncke@mbi-berlin.c
Christian	Weststrate	AMOLF	Netherlands	c.weststrate@amolf.nl
Sander	Woutersen	University of Amsterdam	Netherlands	s.woutersen@uva.nl
Ann Marie	Woys	UW Madison	United States	woys@wisc.edu
Klaas	Wynne	University of Strathclyde	United Kingdom	klaas.wynne@phys.str
Xiaoliang	Xie	Harvard University	United States	xie@chemistry.harvarc
Amanda	Yarnell	American Chemical Society	United States	a_yarnell@acs.org
Martin	Zanni	University of Wisconsin-Madison	United States	zanni@chem.wisc.edu
Larry	Ziegler	Boston University	United States	lziegler@bu.edu
Wolfgang	Zinth	University of Munich	Germany	zinth@physik.uni-mue

## Saturday, May 09, 2009

3:00 PM *Registration*6:00 PM *Reception*

Sponsored by Infrared Systems Development and Infrared Associates

## Sunday, May 10, 2009

7:30 AM *Breakfast*8:50 AM *Opening Remarks*

Andrei Tokmakoff, MIT

9:00 AM *Water and Hydrogen Bonding*

Presiding: Minhaeng Cho, Korea University

9:00 AM In T. Elsaesser, L. Szyc, M. Yang, J. R. Dwyer, E. T. J. Nibbering, *Max-Born Institute**Ultrafast vibrational dynamics of hydrated DNA*9:40 AM C H.J. Bakker, C. Petersen, K.-J. Tielrooij, *AMOLF**Melting of hydrophobic icebergs*10:00 AM C Damien Laage, Guillaume Stirnemann, James T. Hynes, *Ecole Normale Supérieure**Why water reorientation slows down without iceberg formation around hydrophobic solutes*10:20 AM C Artem A. Bakulin, Wayne Liang, Thomas la Cour Jansen, Douwe A. Wiersma, Huib J. Bakker, Maxim S. Pshenichnikov, *Univ. Groningen**Do hydrophobic groups stabilize the water structure?*10:40 AM *Break*11:10 AM *Biochemical Dynamics*

Presiding: Minhaeng Cho, Korea University

11:10 AM In Richard A. Mathies, Renee R. Frontiera, Chong Fang, Jyotishman Dasgupta, Mark Creelman, Sangdeok Shim, *UC Berkeley**Femtosecond Stimulated Raman Spectroscopy of Chemical and Biochemical Reaction Dynamics*11:50 AM C W. Zinth, W. J. Schreier, J. Kubon, N. Regner, K. Haider, T. E. Schrader, P. Clivio, P. Gilch, *University of Munich**Ultrafast IR-spectroscopy: CPD-photodamage in DNA is formed from the excited singlet state*12:10 PM C Allison Stelling, Minako Kondo, Allison Haigney, Ian Clark, Adeibert Bacher, Peter J. Tonge, Stephen R. Meech, *University of East Anglia**Early Events in the Blue-Light Sensing BLUF Domain Protein Viewed Through Time Resolved IR*12:30 PM *Lunch*2:00 PM *Chemical Dynamics*

Presiding: Kevin Kubarych, Univ. of Michigan

2:00 PM C S. Takeuchi, S. Ruhman, T. Tsuneda, M. Chiba, T. Taketsugu, T. Tahara, *RIKEN**Observing continuous structural change of reacting molecules: ISRS and computational study on the reaction coordinate of photoisomerization of cis-stilbene*2:20 PM C Jaane Seehusen, Jorg Lindner, Dirk Schwarzer, and Peter Vohringer, *University of Bonn**Ultrafast vibrational dynamics of artificial hydrogen-bond networks*2:40 PM C M. Panman, P. Bodis, B.H. Bakker, A.M. Brouwer, W.J. Buma, E.R. Kay, D.A. Leigh, S. Woutersen, *University of Amsterdam**Real-time observation of shuttling molecular devices*3:00 PM C Karin Haider, Thorben Cordes, Teja Herzog, Gehad Zeyat, Karola Ruck-Braun, and Wolfgang Zinth, *Lehrstuhl für BioMolekulare Optik**The Photochemistry of Chromenes Studied with Time-Resolved Infrared Spectroscopy*3:20 PM *Break*

Sponsored by Tokyo Instruments

3:50 PM *Multidimensional Spectroscopy*

Presiding: Kevin Kubarych, Univ. of Michigan

3:50 PM In Shaul Mukamel, Oleksiy Roslyak, Cyril Falvo, and Benoit Palmieri*Time Resolved Stimulated Vibrational Spectroscopy with pulse shaping and entangled photons*4:30 PM C Igor V. Rubtsov, Valeriy M. Kasyanenko, Grigory I. Rubtsov, Christopher Keating, Zhiwei Lin, *Tulane University**Correlating Energy Transport Time with Distance using Relaxation-Assisted 2DIR*4:50 PM C Patrick F. Tekavec, Jeffrey A. Myers, Kristin L. M. Lewis, Franklin Fuller, Jennifer P. Ogilvie, *University of Michigan-Ann Arbor**Two-dimensional electronic spectroscopy with a continuum probe*6:00 PM *Dinner*7:30 PM *Poster Session 1*

## Monday, May 11, 2009

7:30 AM *Breakfast*

9:00 AM *Imaging and Single Molecules*

Presiding: Andrei Tokmakoff, MIT

9:00 AM In X. Sunney Xie, Christian W. Freudiger, Wei Min, Brian G. Saar, *Harvard University*

*Label-Free Biomedical Imaging with High Sensitivity by Stimulated Raman Scattering Microscopy*

9:40 AM In J. A. Dieringer, K. L. Wustholz, J. P. Camden, S. L. Kleinman, D. J. Masiello, Y. Wang, R. B. Lettan, K. Scheidt, L. Marks, G. C. Schatz, R. P. Van Duyne, *Northwestern University*

*Advances in Single-Molecule Surface-Enhanced Raman Spectroscopy*

10:20 AM *Break*

Sponsored by Renishaw

10:50 AM *Emerging Methods*

Presiding: John Asbury, *Pennsylvania State University*

10:50 AM In Hanju Rhee and Minhaeng Cho, *Korea University*

*Ultrafast characterization of vibrational optical activity*

11:30 AM C Jan Helbing and Matthias Bonmarin, *Universitat Zurich*

*Transient Vibrational Circular Dichroism Spectroscopy*

11:50 AM C Kristina Wilson, Brendon Lyons, David McCamant, *University of Rochester*

*Two-dimensional stimulated Raman spectroscopy: New developments in theory and experiments that probe intra- and inter-molecular anharmonicity*

12:10 PM C T. Buckup, J. Mohring, M. Motzkus, *Philipps University Marburg*

*Pump-DFWM as multidimensional method to investigate molecular vibrations in the excited state of biological molecules*

12:30 PM *Lunch*

2:00 PM *Ultrafast Dynamics*

Presiding: Munira Khalil, *University of Washington*

2:00 PM In Oshrat Bismuth, Amir Wand, Noga Friedman, Mordechai Sheves, Stanford Ruhman, *Hebrew University*

*Investigating the excited state of the retinal protein chromophore with transient impulsive Raman*

2:40 PM In D. Vorobyev, D. Kuroda, F. Kuo, R. M. Hochstrasser, *University of Pennsylvania*

*Ultrafast IR studies of aqueous ions*

3:20 PM *Break*

Sponsored by ThermoElectron

3:50 PM *Charge Transfer*

Presiding: Munira Khalil, *University of Washington*

3:50 PM C Katrin Adamczyk, Mirabelle Premont-Schwarz, Jens Dreyer, Dina Pines, Ehud Pines, Erik T.J. Nibbering, *Max Born Institut*

*Ultrafast aqueous protonation dynamics of cyanate and bicarbonate*

4:10 PM C Ryan D. Pensack, Kyle M. Banyas, John B. Asbury, *Pennsylvania State University*

*2D IR Spectroscopic Study of Charge Traps in Organic Photovoltaic Polymer Blends*

4:30 PM C Chantelle Anfuso-Cleary, Tianquan Lian, *Emory University*

*Vibrational Sum-Frequency Generation Study of Interfacial Charge Transfer Complexes of Single Crystal TiO<sub>2</sub> Surfaces*

4:50 PM C Sean T. Roberts, Poul B. Petersen, Krupa Ramasesha, and Andrei Tokmakoff, *MIT*

*Transport of the Aqueous Hydroxide Ion Probed Through Ultrafast Two-Dimensional Infrared Spectroscopy*

6:00 PM *Dinner*

7:30 PM *2D IR spectroscopy*

Presiding: Thomas Elsaesser, *Max Born Institute*

7:30 PM In M. D. Fayer, J. Zheng, H. Ishikawa, D. E. Mollanen, K. Kwak, D. E. Rosenfield, *Stanford University*

*Investigations of Chemical Dynamics with Ultrafast 2D IR Vibrational Echo Chemical Exchange Spectroscopy*

8:10 PM In Martin Zanni, *University of Wisconsin-Madison*

*Residue-by-residue structural and time resolution with pulse shaping 2D IR spectroscopy and isotope labeled peptides*

## Tuesday, May 12, 2009

7:30 AM *Breakfast*

9:00 AM *Imaging and Single Molecules*

Presiding: Jennifer Ogilvie, *University of Michigan*

9:00 AM In Hiro-o Hamaguchi, *University of Tokyo*

*Toward single molecule and single cell time-resolved vibrational spectroscopy*

9:40 AM In Gilad Haran, *Weizmann Institute of Science*

*Single-Molecule Raman Scattering: from Plasmonics to Charge Transfer*

10:20 AM C H. Peter Lu, Yuanmin Wang, *Bowling Green State University*

*AFM-Raman Imaging Analysis of Single-Molecule Interfacial Electron Transfer Dynamics*



10:40 AM	<b>Break</b>		
11:10 AM	<b>Spectroscopy at Interfaces</b>		Presiding: Jennifer Ogilvie, <i>University of Michigan</i>
11:10 AM	In	Jeffrey A. Carter, Zhaohui Wang, Alexei Lagutchev, <u>Dana D. Diott</u> , <i>University of Illinois-Urbana Champaign</i>	<i>Dynamics at interfaces probed by time-resolved sum-frequency generation spectroscopy</i>
11:50 AM	C	Yi Rao, Nicholas J. Turro, <u>Kenneth B Eisenthal</u> , <i>Columbia University</i>	<i>Time Resolved Vibrational Sum Frequency Generation (SFG) at Liquid Surfaces</i>
12:10 PM	C	Juraj Bdzoch, Jan Zacharias, Martin Wolf, <u>Christian Frischkorn</u> , <i>Freie Universitat Berlin</i>	<i>Vibrational response of D2O molecules in thin layers absorbed on Ru(001) after femtosecond UV excitation</i>
12:30 PM	<b>Lunch</b>		
2:00 PM	<b>Proteins</b>		Presiding: Stephen Meech, <i>University of East Anglia</i>
2:00 PM	C	<u>Paul M. Champion</u> , <i>Northeastern University</i>	<i>Recent Studies of Coherent Vibrational Motion in Biomolecules</i>
2:20 PM	C	<u>Carsten Kötting</u> , Klaus Gerwert, <i>Ruhr-Universitat Bochum</i>	<i>Proteins in Action: Monitored by tr(time-resolved) FTIR spectroscopy</i>
2:40 PM	C	<u>Ziad Ganim</u> , Kevin Jones, Andrei Tokmakoff, <i>MIT</i>	<i>2D IR Spectroscopy of Insulin Dimer Dissociation and Unfolding Dynamics</i>
3:00 PM	<b>Break</b>		
3:30 PM	<b>Multidimensional Spectroscopy</b>		Presiding: Stephen Meech, <i>University of East Anglia</i>
3:30 PM	C	<u>Charles B. Harris</u> , James F. Cahoon, Karma R. Sawyer, Jacob P. Schlegel, Matthew C. Zorb, <i>University of California-Berkeley</i>	<i>Using two dimensional vibrational spectroscopy to determine transition state geometries in liquids</i>
3:50 PM	C	Michael Lynch, Mark Cheng, Benjamin Van Kuiken, <u>Munira Khalil</u> , <i>University of Washington-Seattle</i>	<i>Understanding vibrational interactions on the ground and electronic excited states of transition metal complexes using multidimensional visible-infrared spectroscopies</i>
4:10 PM	C	Carlos R. Baiz, Matthew J. Nee, Robert McCanne, <u>Kevin J. Kubarych</u> , <i>University of Michigan</i>	<i>Temperature-dependent vibrational relaxation measured by non-equilibrium 2DIR spectroscopy</i>
4:30 PM	C	A.I. Stewart, R. Kania, G.M. Greetham, I.P. Clark, M. Towrie, A.W. Parker, <u>N.T. Hunt</u> , <i>University of Strathclyde</i>	<i>Vibrational Dynamics of a Free Radical Intermediate via Transient 2D-IR Spectroscopy of a Photolysis Reaction</i>
6:00 PM	<b>Dinner</b>		
7:30 PM	<b>Poster Session 2</b>		

## Wednesday, May 13, 2009

7:30 AM	<b>Breakfast</b>		
9:00 AM	<b>Water and Peptides</b>		Presiding: Huib Bakker, <i>AMOLF</i>
9:00 AM	In	<u>Jim Skinner</u> , <i>University of Wisconsin-Madison</i>	<i>Water and peptide structure and dynamics as probed by vibrational spectroscopy</i>
9:40 AM	C	V.V. Volkov, <u>R. Righini</u> , <i>University of Florence</i>	<i>Structural properties and dynamics of membrane associated anchor peptide</i>
10:00 AM	C	<u>Ellen Backus</u> , Robbert Bloem, Peter Hamm, <i>FOM Institute for Atomic and Molecular Physics</i>	<i>Glass transition regulated heat transport through a helical peptide</i>
10:20 AM	C	<u>Thomas la Cour Jansen</u> , Chungwen Liang, Jasper Knoester, <i>University of Groningen</i>	<i>Isotope label 2DIR spectroscopy in proteins</i>
10:40 AM	<b>Break</b>		
11:10 AM	<b>Solid State and Terahertz</b>		Presiding: Huib Bakker, <i>AMOLF</i>
11:10 AM	C	Matthias C. Hoffmann, Janos Hebling, Harold Y. Hwang, Ka-Lo Yeh, <u>Keith A. Nelson</u> , <i>MIT</i>	<i>THz-pump/THz-probe nonlinear spectroscopy</i>
11:30 AM	C	<u>Tomonori Nomoto</u> and Hiroshi Onishi, <i>Kobe University</i>	<i>Near-surface low-frequency vibrations of TiO2 observed by fourth-order coherent Raman spectroscopy</i>
11:50 AM	C	J. Mance, F.X. Morrissey, <u>S.L. Dexheimer</u> , <i>Washington State University</i>	<i>Acoustic and optical phonon dynamics in excitation self-trapping</i>
12:10 PM	C	<u>C. Konek</u> , J. Wilkinson, J. Hooper, O. Esenturk, E. Heilweil, <i>Indian Head, Naval Surface Warfare Center</i>	<i>Terahertz Spectroscopy of Explosives</i>
12:30 PM	<b>Lunch</b>		

2:00 PM		<i>Vibrational Dynamics in Liquids</i>	Presiding: Edwin Heilweil, <i>NIST</i>
2:00 PM	C	<u>Takayoshi Kobayashi</u> , Izumi Iwakura, and Atsushi Yabushita, <i>University of Electro-Communications</i>	<i>Direct observation of molecular structural change during oxidation in the ground state triggered by stimulated Raman by a 5fs laser</i>
2:20 PM	C	<u>A. Paarmann</u> , M. Lima, R. Chelli, V. V. Volkov, R. Righini, R. J. D. Miller, <i>University of Toronto</i>	<i>Vibrational Excitons in Liquid Formamide</i>
2:40 PM	C	David A. Turton and <u>Klaas Wynne</u> , <i>University of Strathclyde</i>	<i>Ultrafast cage rattling and TA "phonon" modes in atomic and molecular liquids: implications for glass formation</i>
5:30 PM		<i>Excursion and Banquet</i>	

#### Thursday, May 14, 2009

7:30 AM		<i>Breakfast</i>	
9:00 AM		<i>Peptides and Proteins</i>	Presiding: Tahei Tahara, <i>RIKEN</i>
9:00 AM	C	<u>Esben Ravn Andresen</u> and Peter Hamm, <i>Universitat Zurich</i>	<i>Site-specific difference 2D-IR spectroscopy of bacteriorhodopsin</i>
9:20 AM	C	<u>Mariangela Di Donato</u> , L.J.G.W. van Wilderen, Klaas Hellingwerf, Ivo H.M. Van Stokkum, Rienk van Grondelle, Marie Louise Groot, <i>Vrije Universiteit Amsterdam</i>	<i>The proton transfer pathway in Green Fluorescent Proteins studied with femtosecond time resolved Vis/midIR pump-probe spectroscopy and multi-pulse visible spectroscopy</i>
9:40 AM	C	C. Krejtschi, O. Ridderbusch, R. Huang, L. Wu, T.A. Keiderling, <u>K. Hauser</u> , <i>University of Frankfurt</i>	<i>Site-specific folding dynamics of peptides studied by temperature-jump infrared-spectroscopy</i>
10:00 AM	C	<u>Hajime Torii</u> , <i>Shizuoka University</i>	<i>Toward Efficient Time-Domain Calculations of 2D-IR Spectra</i>
10:20 AM	C	<u>van Thor JJ</u> , Ronayne KL, Towrie M, Sage JT, <i>Imperial College London</i>	<i>Balance between ultrafast parallel reactions in the green fluorescent protein has a structural origin</i>
10:40 AM		<i>Break</i>	
11:10 AM		<i>Water at Interfaces</i>	Presiding: Tahei Tahara, <i>RIKEN</i>
11:10 AM	In	<u>Mischa Bonn</u> , <i>FOM-Institute for Atomic and Molecular Physics</i>	<i>Structure and dynamics of interfacial water</i>
11:50 AM	C	I.V. Stiopkin, C. Weeraman, F. Shalhout, <u>A.V. Benderskii</u> , <i>Wayne State University</i>	<i>Vibrational Line Shapes and Ultrafast Orientational Dynamics at the Air/Water Interface</i>
12:10 PM	C	Ali Eftekhari-Bafrooei and <u>Eric Borguet</u> , <i>Temple University</i>	<i>The effect of ordering on the vibrational dynamics of interfacial water</i>
12:30 PM		<i>Lunch</i>	

Authors	Title
<b>Sunday, May 10, 2009</b>	
1 <u>Sean Garrett-Roe</u> and Peter Hamm, <i>University of Zurich</i>	<i>3D-IR of isotopically substituted water (HOD/H<sub>2</sub>O) and CO<sub>2</sub> in water</i>
2 <u>Krupa Ramasesha</u> , Sean T. Roberts, Andrei Tokmakoff, <i>MIT</i>	<i>Anisotropy of Water studied using Molecular Dynamics Simulations</i>
3 <u>Guillaume Stirnemann</u> , Peter J. Rossky, James T. Hynes, Damien Laage, <i>Ecole Normale Supérieure</i>	<i>Water Reorientation and Hydrogen-Bond Dynamics next to an Extended Hydrophobic Surface</i>
4 <u>Y.-S. Lin</u> and J. L. Skinner, <i>University of Wisconsin-Madison</i>	<i>Ultrafast Infrared Spectroscopy of Dilute HOD in Aqueous Salt solutions</i>
5 <u>Junichi Ono</u> , Yoshitaka Tanimura, Shinji Saito, <i>Kyoto University</i>	<i>A Theoretical Study of Intermolecular Vibrational Mode Coupling in Aqueous Solutions</i>
6 Daniel Shaw, <u>Matthijs Panman</u> , Sander Woutersen, <i>University of Amsterdam</i>	<i>Cooperative vibrational relaxation in hydrogen-bonded liquids</i>
7 <u>Lukasz Piatkowski</u> , Huib Bakker, <i>AMOLF</i>	<i>Ultrafast intermolecular energy transfer in heavy water</i>
8 Thomas la Cour Jansen, Dan Cringus, <u>Maxim S. Pshenichnikov</u> , <i>University of Groningen</i>	<i>Dynamics of Water Symmetric-Asymmetric Stretches</i>
9 <u>Rebecca A. Nicodemus</u> and Andrei Tokmakoff, <i>MIT</i>	<i>Temperature Dependent 2D IR and Pump Probe Measurements of HOD in H<sub>2</sub>O</i>
10 <u>Scott M. Gruenbaum</u> , Roger F. Loring, <i>Cornell University</i>	<i>Interference and Quantization in Semiclassical Response Functions</i>
11 <u>Sean T. Roberts</u> , Poul B. Petersen, Krupa Ramasesha, and Andrei Tokmakoff, <i>MIT</i>	<i>Transport of the Aqueous Hydroxide Ion Probed Through Ultrafast Two-Dimensional Infrared Spectroscopy</i>
12 <u>Poul B. Petersen</u> , Sean T. Roberts, Krupa Ramasesha, Daniel G. Nocera and Andrei Tokmakoff, <i>MIT</i>	<i>Vibrational Dynamics of Proton Transfer Systems</i>
13 <u>R.L.A. Timmer</u> , M.J. Cox, H.J. Bakker, <i>AMOLF</i>	<i>Proton transfer in ice</i>
14 V. Kozich, J. Dreyer, <u>W. Werncke</u> , <i>Max Born Institut</i>	<i>Mode-selective vibrational redistribution after spectrally selective N-H stretching mode excitation in intermolecular hydrogen bonds</i>
15 <u>Feng Ding</u> , Qin Zhong, Michael R. Brindza, Robert A. Walker, John T. Fourkas, <i>University of Maryland at College Park</i>	<i>Surface studies of liquids using counter-propagating vibrational sum frequency spectroscopy</i>
16 <u>Patrick L. Hayes</u> , Ehow H. Chen, Jennifer L. Achtyl, Franz M. Geiger, <i>Northwestern University</i>	<i>Tracking Charge Densities and Conformations of a Cationic Surfactant at Silica/Aqueous Interfaces with Vibrational Sum Frequency Generation</i>
17 Jorg Lindner, Tim Schafer, Dirk Schwarzer, <u>Peter Vohringer</u> , <i>University of Bonn</i>	<i>Vibrational energy relaxation in liquid-to-supercritical ammonia</i>
18 <u>David Turton</u> , Klaas Wynne, <i>University of Strathclyde</i>	<i>Observation of mesoscopic structure in ionic liquids by ultrafast OKE and dielectric spectroscopies</i>
19 <u>I.A. Heisler</u> and S.R. Meech, <i>University of East Anglia</i>	<i>Ultrafast Liquid Dynamics Under Strain</i>
20 <u>Daniel Shaw</u> and Sander Woutersen, <i>University of Amsterdam</i>	<i>Non-dipolar resonant intermolecular energy transfer in hydrogen bonded liquids</i>
21 <u>K. Mazur</u> , I. A. Heisler, S. R. Meech, <i>University of East Anglia</i>	<i>Unraveling the Raman Spectral Density of Complex Fluids with Diffractive Optics OKE Measurements</i>
22 <u>Rintaro Shimada</u> , Hiro-o Hamaguchi, <i>University of Tokyo</i>	<i>Selective detection of proximate solvent molecules by the molecular near-field effect in resonance hyper-Raman scattering</i>
23 <u>S.D. McGrane</u> , R.J. Scharff, M. Greenfield, and D.S. Moore, <i>Los Alamos National Laboratory</i>	<i>Pulse shaping of filamentation broadened pulses for optimizing coherent Raman spectroscopy</i>
24 Meng Cui, Brandon R. Bachler, Sarah R. Nichols and <u>Jennifer P. Ogilvie</u> , <i>University of Michigan-Ann Arbor</i>	<i>A Comparison Between Coherent and Spontaneous Raman Scattering Under Biological Imaging Conditions</i>

- 25 **M. Liu**, B. Pardo, M.M. Qazilbash, S.J. Yun, B.G. Chae, B.J. Kim, D.N. Basov, R.D. Averitt, *Boston University* *Conductivity Dynamics in the Correlated Metallic State of  $V_2O_3$*
- 26 **Artem A. Bakulin**, Dmitry Yu. Paraschuk, Paul H.M. van Loosdrecht, and Maxim S. Pshenichnikov, *University of Groningen* *Ground-state charge-transfer complexes of conjugated polymer as an intermediate for charge photogeneration*
- 27 **Aaron M. Massari**, Audrey A. Eigner, *University of Minnesota* *1D and 2D-IR spectroscopy of blended polymer-porphyrin thin films*
- 28 **T. Buckup**, J. Mohring, M. Motzkus, *Philipps University Marburg* *Manipulating vibrational wavepackets with direct UV shaping*

## Tuesday, May 12, 2009

- 1 **Jessica M. Anna**, Kevin J. Kubarych, *University of Michigan-Ann Arbor* *Equilibrium dynamics of dicobalt octacarbonyl: the effects of isomerization on coherences*
- 2 **Robert McCanne**, Carlos Baiz, Matthew J. Nee, Jessica Anna, Kevin J. Kubarych, *University of Michigan-Ann Arbor* *Using Transient Fourier Transform Two-Dimensional Infrared Spectroscopy to Monitor Non-Equilibrium Reactions and Dynamics*
- 3 **Carlos R. Baiz**, Kevin J. Kubarych, *University of Michigan-Ann Arbor* *Intermolecular vibrational energy transfer studies with non-equilibrium infrared photon echo spectroscopy*
- 4 **Nadja Regner**, Thorben Cordes, Karin Haiser, Karola Ruck-Braun, Wolfgang Zinth, *LMU Munchen* *Dynamics of Photoswitchable Hemithioindigo-Peptides*
- 5 **Koichi Iwata**, Nobuyuki Asami, Tomohisa Takaya, James Calladine, Xue-Zhong Sun, Michael W. George, Antony W. Parker, Soshi Yabumoto, Shinsuke Shigeto, Hiro-o Hamaguchi, *University of Tokyo* *Mechanism of ultrafast charge transfer reaction in 9,9'-bianthryl examined with time-resolved mid-infrared and near-infrared spectroscopy*
- 6 Katrin Adamczyk, Natalie Banerji, **Bernhard Lang**, Omar F. Mohammend, Erik T. J. Nibbering, Eric Vauthey, *University of Geneva* *Tight and loose ion pairs as primary reaction products of highly exergonic photo-induced bimolecular electron transfer*
- 7 **Sergey V. Shilov**, Thomas J. Tague, *Bruker Optics* *Time-resolved step-scan FTIR spectroscopy with a new research vacuum spectrometer*
- 8 **Kevin C. Jones**, Ziad Ganim, Andrei Tokmakoff, *MIT* *Heterodyned Detection for Linear and Nonlinear Infrared Signal Characterization*
- 9 **Michael Lynch**, Mark Cheng, Benjamin Van Kuiken, and Munira Khalil, *University of Washington* *Understanding vibrational interactions on the ground and electronic excited states of transition metal complexes using multidimensional visible-infrared spectroscopies*
- 10 **Zhiwei Lin**, Valeriy M. Kasyanenko, Grigory I. Rubtsov, Igor V. Rubtsov, *Tulane University* *Interferometric delay measurements implemented for dual-frequency 2DIR setup*
- 11 **Hideaki Kano** and Hiro-o Hamaguchi, *University of Tokyo* *Time-resolved CARS imaging of cell division using a supercontinuum light source*
- 12 **Jan. Helbing**, Harald. Bregy, Peter Hamm, *Universitat Zurich* *Parameters governing the transient 2D-IR spectra of peptides - the opening of a beta turn thioxopeptide*
- 13 **Joshua Lessing**, Jongjin Kim, Kevin Jones, Ziad Ganim, and Andrei Tokmakoff, *MIT* *Two dimensional vibrational spectroscopy study of hydrophobic collapse in bovine neck elastin and elastin like proteins*
- 14 **Ann Marie Woys**, Martin T. Zanni, *University of Wisconsin-Madison* *2D IR Spectroscopy of native probes provide clues to the structure of peptides in a lipid bilayer*
- 15 **L.D. Ziegler**, L. R. Chieffo, J. T. Shattuck, E. Pinnick, F. Wang, S. Erramilli, *Boston University* *Nitrous oxide vibrational relaxation: A probe of interfacial water in phospholipid bilayers*
- 16 Eeva-Liisa Karjalainen, **Andreas Barth**, *Stockholm University* *Analysis of protein backbone structural changes by experiment and calculation*
- 17 **Kyriil M. Solntsev**, Laren M. Tolbert, *Georgia Institute of Technology* *Excited-state proton transfer in novel photoacids: Introducing a challenge for the TRVS studies*
- 18 **Karsten Neumann**, Mirka-Kristin Verhoeven, Gabreila Schafer, Georg Wille, Werner Mantele, Josef Wachtveitl, *Johann Wolfgang Goethe University Frankfurt/Main* *Nitrophenylacetate anion as caged compound for  $CO_2$ : direct observation of the photodecarboxylation*

- 19 Andreas D. Stahl, Mariangela Didonato, Ivo van Stokkum, Marie Louise Groot, *VU University Amsterdam* *Excitation Energy Transfer in PS1 and LHC2 measured in the midIR: Spectroscopy & Structural Relations*
- 20 M. Yoshizawa, D. Kosumi, R. Nakamura, Y. Iwabuchi, M. Fujiwara, and H. Hashimoto, *Tohoku University* *Vibrational dynamics of the dark excited state (S1) in beta-Carotene investigated by two-photon excitation spectroscopy*
- 21 Sergei G. Kruglik, Jean-Louis Martin, Michel Negre, *Ecole Polytechnique* *Measurement of domed-to-planer heme motion induced by NO binding to myoglobin*
- 22 J.C. Owrutsky, D.J. Brown, G.M. Sando, *Naval Research Laboratory* *Vibrational dynamics of molecular and networked metal cyanides*
- 23 Christopher Keating, Sriram G. Naraharisetty, Beth A. McClure, Jeff Rack, Igor V. Rubtsov, *Tulane University* *The Use of Sulfoxides as Structural Reporters in Dual-Frequency 2DIR Spectroscopy*
- 24 M. Candelaresi, M. Pagliai, M. Lima, P. Foggi, R. Righini, *University of Florence* *Solvation dynamics of methyl acetate probed by two-dimensional IR spectroscopy*
- 25 G. Seifert, S. Arnold, H. Graener, *Martin-Luther-Universität Halle-Wittenberg* *Vibrational energy relaxation of halogenated methane derivatives of the type CHX<sub>3</sub> and CH<sub>2</sub>X<sub>2</sub> (X=Cl, Br, J)*
- 26 Valeriy M. Kasyanenko, Zhiwei Lin, Grigory I. Rubtsov, James P. Donahue, Igor V. Rubtsov, *Tulane University* *Energy Transport Between Ligands in Transition Metal Complexes*